

4/5/1

DIALOG(R) File 303:Chapman & Hall Chemical Database
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01121222

Subfile: Dictionary of Drugs, 1990;Dictionary of Steroids, 1991;Dictionary of Organic Compounds, 6th Edn., 1996;Dictionary of Pharmacological Agents, 1997

CHCD Acc. No: L-00049K0;L-00036J0;L-000096A20;L-00101X0

Unique Key: 00353351- -00

CHCD NAME: Lilopristone

Synonyms: 1-[4-(Dimethylamino)phenyl]-17-hydroxy-17-(3-hydroxy-1-propenyl)estradi-4,9-dien-3-one ; ZK 98734

Compound Type: Selected General Organics - Nonaromatic 19-norandrostane steroids (estranes) (C18); Pharmacological Agents - Abortifacients

Use/Importance: Abortifacient

Physical State: Pale-yellow foam

CAS Registry No: 97747-88-1

Molecular Formula: C₂₉H₃₇NO₃

Molecular Wt: 447.616

RTECS No.: KG2940000

Optical Rotation: +203.5 deg (CHCl₃) wavelength Na line

References:

01A GP 1985 3 347 126

01B CA 104 186715 (synth)

Data Tags: CAS Registry number; Molecular formula; Use/Importance; Physical State; Optical Rotation; RTECS Reference

4/5/2

DIALOG(R) File 303:Chapman & Hall Chemical Database

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00433714

Subfile: Dictionary of Drugs, 1990;Dictionary of Steroids, 1991;Dictionary of Organic Compounds, 6th Edn., 1996;Dictionary of Pharmacological Agents, 1997

CHCD Acc. No: L-00049K0;L-00036J0;L-000096A20;L-00101X0

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Optical Rotation: +203.5 deg (CHCl₃) wavelength Na line

References:

01A Ger. Pat. 1985 3 347 126

01B CA 104 186715 (synth)

Data Tags: CAS Registry number; Molecular formula; Use/Importance; Physical State; Optical Rotation; RTECS Reference

?

107217911 CA: 107(23)217911k JOURNAL

Synthesis of

11.beta.- (4-dimethylaminophenyl)-17.beta.-hydroxy-17.alpha.- (1-propynyl) est
ra-4,9-dien-3-one (RU-486)

AUTHOR(S): Chen, Lianzhi; Sheng, Shi; Fang, Xiuru; Yang, Xiao; Chen,
Beining; Shi, Jufang; Liu, Caixia; Peng, Sixun

LOCATION: Dep. Pharm. Chem., Nanjing Coll. Pharm., Nanjing, Peop. Rep.
China,

JOURNAL: Nanjing Yaoxueyuan Xuebao DATE: 1986 VOLUME: 17 NUMBER: 4

PAGES: 282-5 CODEN: NYXUDF ISSN: 0254-5055 LANGUAGE: Chinese

SECTION:

CA232003 Steroids

IDENTIFIERS: RU 486, estradienone dimethylaminophenylhydroxypropynyl
CAS REGISTRY NUMBERS:

7353-91-5 32423-84-0 Grignard reaction of, with estradienone deriv.

899-79-6P prepn. and cyclization of

1089-78-7P prepn. and dehydrogenation of

84371-64-2P prepn. and deketalization of

84371-69-7P prepn. and epoxidn. of

84371-57-3P prepn. and Grignard reaction of, with (dimethylamino)phenyl
magnesium bromide

966-47-2P 6733-79-5P prepn. and hydrogenation of

6218-29-7P prepn. and ketalization of

1091-93-6P prepn. and oxidative demethylation of

53303-91-6P prepn. and oxidn. of

5571-36-8P prepn. and propynylation of

1035-77-4P 1624-62-0P 6885-44-5P prepn. and redn. of

84371-65-3P prepn. of

111058-54-9 reaction of, with methylcyclopentanedione deriv.

8/5/7
DIALOG(R) File 399:CA SEARCH(R)
(c) 1998 American Chemical Society. All rts. reserv.

74010081 CA: 74(3)10081u JOURNAL
Orally active long-acting estrogen (AY-20,121)
(3-(2-propynloxy)-estra-1,3,5(10)-trien-17.beta.-ol trimethylacetate)
AUTHOR(S): Banik, Upendra K.; Revesz, Clara; Herr, Ferenc
LOCATION: Ayerst Res. Lab., Montreal, Que.
JOURNAL: Steroids DATE: 1970 VOLUME: 16 NUMBER: 3 PAGES: 289-96
CODEN: STEDAM LANGUAGE: English

SECTION:

CA804000 Hormones and Related Substances
IDENTIFIERS: estrogens synthetic, contraceptives steroids

DESCRIPTORS:

Estrogenic hormones...
(propynloxy)estratrienol trimethylacetate

Vagina...
(propynloxy)estratrienol trimethylacetate effect on epithelium of

CAS REGISTRY NUMBERS:

57-63-6 152-43-2 biol. activity of, (propynloxy)estratrienol
trimethylacetate in relation to
28002-65-5 estrogenic hormone

8/5/1

DIALOG(R) File 399:CA SEARCH(R)

(c) 1998 American Chemical Society. All rts. reserv.

120096113 CA: 120(9)96113j JOURNAL

Biotransformation of

17.beta.-hydroxy-11.beta.-(4-dimethylaminophenyl)17.alpha.-1-propynyl-estra
-4,9-dien-3-one (RU486) in rat hepatoma variants

AUTHOR(S): Chasserot-Golaz, S.; Beck, G.; Venetianer, A.

LOCATION: Unite Propre Recherche, CNRS, 67000, Strasbourg, Fr.

JOURNAL: Biochem. Pharmacol. DATE: 1993 VOLUME: 46 NUMBER: 11 PAGES:
2100-3 CODEN: BCPCA6 ISSN: 0006-2952 LANGUAGE: English

SECTION:

CA202004 Mammalian Hormones

CA201XXX Pharmacology

IDENTIFIERS: RU486 metab liver cytochrome P450

DESCRIPTORS:

Liver, neoplasm, hepatoma...

Reuber, RU486 metab. by, CYP3A involvement in

CAS REGISTRY NUMBERS:

9035-51-2 biological studies, CYP3A, in RU486 metab. by hepatoma

9035-51-2 biological studies, in RU486 metab. by hepatome

84371-65-3 metab. of, by hepatoma

8/5/2

DIALOG(R) File 399:CA SEARCH(R)

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107217911 CA: 107(23)217911k JOURNAL

Synthesis of

11.beta.- (4-dimethylaminophenyl)-17.beta.-hydroxy-17.alpha.- (1-propynyl) est
ra-4,9-dien-3-one (RU-486)

AUTHOR(S): Chen, Lianzhi; Sheng, Shi; Fang, Xiuru; Yang, Xiao; Chen,
Beining; Shi, Jufang; Liu, Caixia; Peng, Sixun

LOCATION: Dep. Pharm. Chem., Nanjing Coll. Pharm., Nanjing, Peop. Rep.
China,

JOURNAL: Nanjing Yaoxueyuan Xuebao DATE: 1986 VOLUME: 17 NUMBER: 4

PAGES: 282-5 CODEN: NYXUDF ISSN: 0254-5055 LANGUAGE: Chinese

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1089-78-7P prepn. and dehydrogenation of

84371-64-2P prepn. and deketalization of

84371-69-7P prepn. and epoxidn. of

84371-57-3P prepn. and Grignard reaction of, with (dimethylamino)phenyl
magnesium bromide

966-47-2P 6733-79-5P prepn. and hydrogenation of

6218-29-7P prepn. and ketalization of

1091-93-6P prepn. and oxidative demethylation of

53303-91-6P prepn. and oxidn. of

5571-36-8P prepn. and propynylation of

1035-77-4P 1624-62-0P 6885-44-5P prepn. and redn. of

84371-65-3P prepn. of

111058-54-9 reaction of, with methylcyclopentanedione deriv.

8/5/8

DIALOG(R) File 399:CA SEARCH(R)

(c) 1998 American Chemical Society. All rts. reserv.

73056310 CA: 73(11)56310a PATENT

Rodenticidal 3-(2-propynyloxy)-estra-1,3,5(10)-trien-17.beta.-ol pivalate

INVENTOR(AUTHOR): Kruger, Gunther

ASSIGNEE: American Home Products Corp.

PATENT: United States US 3496272 DATE: 700217

APPLICATION: United States DATE: 680123

PAGES: 3 pp. CODEN: USXXAM CLASS: 424-238; A 01n

SECTION:

CA832000 Steroids

IDENTIFIERS: rodenticidal propynyloxy estratrienols

DESCRIPTORS:

19-Norsteroids...

17-hydroxy-3-(2-propynyloxy) pivalate

CAS REGISTRY NUMBERS:

24099-40-9P 24894-50-6P 28002-65-5P 28151-61-3P 28275-48-1P

28275-49-2P 28275-50-5P 28425-85-6P prepn. of

4/5/1

IALOG(R) File 399:CA SEARCH(R)

c) 1998 American Chemical Society. All rts. reserv.

109110741 CA: 109(13)110741u PATENT

11.beta.- (4-Isopropenylphenyl)estra-4,9-dienes, procedure for their
reparation, pharmaceutical preparations containing them, and their use as
antigestagens

INVENTOR(AUTHOR): Ottow, Eckhard; Wiechert, Rudolf; Neef, Guenter; Beier,
Wybille; Elger, Walter; Henderson, David

LOCATION: Fed. Rep. Ger.

ASSIGNEE: Schering A.-G.

PATENT: Germany Offen. ; DE 3625315 A1 DATE: 880128

APPLICATION: DE 3625315 (860725)

PAGES: 5 pp. CODEN: GWXXBX LANGUAGE: German CLASS: C07J-001/00A;
C07C-041/00B; A61K-031/565B; A61K-031/57B; A61K-031/575B

SECTION:

A232003 Steroids

A202XXX Mammalian Hormones

IDENTIFIERS: progesterone antagonist estradiene prepn, antigestagen

estradiene prepn

DESCRIPTORS:

Progesterogens...

inhibitors, estradiene derivs.

Steroids, preparation...

prepn. of estradienes as antigestagens

CAS REGISTRY NUMBERS:

57-83-0 biological studies, antagonists to, estradiene derivs. as

93697-60-0 Grignard reaction of, with bromoisopropenylbenzene

5888-79-5 Grignard reaction of, with epoxyestrenol deriv.

116196-34-0P 116229-17-5P prepn. and reaction of, in synthesis of
antigestagenic estradiene deriv.

116196-21-5P 116196-22-6P 116196-23-7P 116196-24-8P 116196-25-9P

116196-26-0P 116196-27-1P 116196-28-2P 116196-29-3P 116196-30-6P

116196-31-7P 116196-32-8P prepn. of, as antigestagen

8/5/9

IALOG(R) File 399:CA SEARCH(R)

c) 1998 American Chemical Society. All rts. reserv.

72032135 CA: 72(7)32135a PATENT

3-Alkoxy-17.alpha.-propynylestra-1,3,5(10)-trien-17.beta.-ols

INVENTOR(AUTHOR): Galantay, Eugene E.

ASSIGNEE: Sandoz Ltd.

PATENT: Germany Offen. DE 1907330 DATE: 691023

APPLICATION: United States DATE: 680219

PAGES: 20 pp. CODEN: GWXXBX CLASS: C 07c; A 61k

SECTION:

A832000 Steroids

IDENTIFIERS: estratrienols propynyl

DESCRIPTORS:

9-Norsteroids...

3-alkoxy

CAS REGISTRY NUMBERS:

4640-01-5P 24640-02-6P 24640-03-7P 24640-04-8P prep. of

4/5/2

DIALOG(R) File 399:CA SEARCH(R)

(c) 1998 American Chemical Society. All rts. reserv.

106129694 CA: 106(16)129694r JOURNAL

Structure of

11.beta.- (4-(dimethylamino)phenyl)-17.beta.-hydroxy-17.alpha.- (2-propenyl)estradien-3-one

AUTHOR(S): Van Geerestein, V. J.; Kanters, J. A.; Kroon, J.

LOCATION: Lab. Kristal- Structuurchem., Rijksuniv. Utrecht, 3508 TB,
Utrecht, Neth.

JOURNAL: Acta Crystallogr., Sect. C: Cryst. Struct. Commun. DATE: 1987

VOLUME: C43 NUMBER: 2 PAGES: 319-22 CODEN: ACSCEE ISSN: 0108-2701

LANGUAGE: English

SECTION:

CA275008 Crystallography and Liquid Crystals

CA232XXX Steroids

IDENTIFIERS: mol structure methylaminophenylistradienone, estradienone
methylaminophenyl hydroxy propenyl structure, propenylestradienone
structure

DESCRIPTORS:

Crystal structure... Molecular structure...

of ((dimethylamino)phenyl)hydroxypropenylestradienone

CAS REGISTRY NUMBERS:

91935-00-1 crystal structure of

8/5/1

DIALOG(R) File 399:CA SEARCH(R)

(c) 1998 American Chemical Society. All rts. reserv.

120096113 CA: 120(9)96113j JOURNAL

Biotransformation of

17.beta.-hydroxy-11.beta.-(4-dimethylaminophenyl)17.alpha.-1-propynyl-estra
-4,9-dien-3-one (RU486) in rat hepatoma variants

AUTHOR(S): Chasserot-Golaz, S.; Beck, G.; Venetianer, A.

LOCATION: Unite Propre Recherche, CNRS, 67000, Strasbourg, Fr.

JOURNAL: Biochem. Pharmacol. DATE: 1993 VOLUME: 46 NUMBER: 11 PAGES:

2100-3 CODEN: BCPCA6 ISSN: 0006-2952 LANGUAGE: English

SECTION:

CA202004 Mammalian Hormones

CA201XXX Pharmacology

IDENTIFIERS: RU486 metab liver cytochrome P450

DESCRIPTORS:

Liver, neoplasm, hepatoma...

Reuber, RU486 metab. by, CYP3A involvement in

CAS REGISTRY NUMBERS:

9035-51-2 biological studies, CYP3A, in RU486 metab. by hepatoma

9035-51-2 biological studies, in RU486 metab. by hepatome

84371-65-3 metab. of, by hepatoma

8/5/7

DIALOG(R) File 399:CA SEARCH(R)

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74010081 CA: 74(3)10081u JOURNAL

Orally active long-acting estrogen (AY-20,121)

(3-(2-propynloxy)-estra-1,3,5(10)-trien-17.beta.-ol trimethylacetate)

AUTHOR(S): Banik, Upendra K.; Revesz, Clara; Herr, Ferenc

LOCATION: Ayerst Res. Lab., Montreal, Que.

JOURNAL: Steroids DATE: 1970 VOLUME: 16 NUMBER: 3 PAGES: 289-96

CODEN: STEDAM LANGUAGE: English

SECTION:

CA804000 Hormones and Related Substances

IDENTIFIERS: estrogens synthetic, contraceptives steroids

DESCRIPTORS:

Estrogenic hormones...

(propynloxy)estratrienol trimethylacetate

Vagina...

(propynloxy)estratrienol trimethylacetate effect on epithelium of

CAS REGISTRY NUMBERS:

57-63-6 152-43-2 biol. activity of, (propynloxy)estratrienol

trimethylacetate in relation to

28002-65-5 estrogenic hormone

4/5/2

DIALOG(R) File 399:CA SEARCH(R)

(c) 1998 American Chemical Society. All rts. reserv.

106129694 CA: 106(16)129694r JOURNAL

[Structure of

11.beta.- (4-(dimethylamino)phenyl)-17.beta.-hydroxy-17.alpha.- (2-propenyl)estradi-4,9-dien-3-one

AUTHOR(S): Van Geerestein, V. J.; Kanters, J. A.; Kroon, J.

LOCATION: Lab. Kristal- Structuurchem., Rijksuniv. Utrecht, 3508 TB, Utrecht, Neth.

JOURNAL: Acta Crystallogr., Sect. C: Cryst. Struct. Commun. DATE: 1987

VOLUME: C43 NUMBER: 2 PAGES: 319-22 CODEN: ACSCEE ISSN: 0108-2701

LANGUAGE: English

SECTION:

CA275008 Crystallography and Liquid Crystals

CA232XXX Steroids

IDENTIFIERS: mol structure methylaminophenyl estradienone, estradienone methylaminophenyl hydroxy propenyl structure, propenylestradienone structure

DESCRIPTORS:

Crystal structure... Molecular structure...

of ((dimethylamino)phenyl)hydroxypropenylestradienone

CAS REGISTRY NUMBERS:

91935-00-1 crystal structure of

01658020 ORDER NO: AAD98-40400
TUBULIN AS A THERAPEUTIC TARGET (ANGIOGENESIS, CANCER,
COLCHICINE, METHOXYESTRADIOL)

Author: MILLER, THOMAS ALLEN

Degree: PH.D.

Year: 1998

Corporate Source/Institution: UNIVERSITY OF VIRGINIA (0246)

Adviser: TIMOTHY L. MACDONALD

Source: Volume 5907B of Dissertations Abstracts International.

PAGE 3454 . 137 PAGES

Descriptors: CHEMISTRY, ORGANIC ; HEALTH SCIENCES, ONCOLOGY

Descriptor Codes: 0490; 0992

2-Methoxyestradiol, a mammalian metabolite of estradiol, has reported antiangiogenic activity which has been proposed to be mediated through interaction at the colchicine binding site on the tubulin heterodimer. Structure-activity studies of 2-methoxyestradiol have yielded highly potent steroidal inhibitors of tubulin polymerization. Motivated by the potent antiangiogenic activity of 2-Methoxyestradiol and by its ability to inhibit the polymerization of tubulin, either of which may provide therapeutic benefits, our research program has been directed towards the synthesis and characterization of 2-methoxyestradiol derivatives to address critical issues of the biological activity of this estrane class. These efforts seek to establish a greater understanding of the structural relationship between 2-methoxyestradiol and colchicine, and may permit the design of more efficacious hybrid molecules that elicit their activities through the interaction with tubulin. A series of colchicine/2-methoxyestradiol hybrids was synthesized. The A-homo-estrane hybrid systems used in this study, collectively termed estratropes, incorporate structural features of colchicine into the estrane nucleus in an effort to explore the relationship between the antiangiogenic and tubulin binding activities of 2-methoxyestradiol and structure, and the scope of binding at the colchicine binding site. The estratropes were evaluated for their abilities to inhibit the polymerization of tubulin using an in vitro purified bovine brain assay. Several of these hybrids inhibit polymerization with greater potency than either of the natural products. The most potent of these congeners possessed an approximate five-fold enhancement of the activity of colchicine for the inhibition of tubulin polymerization. Additionally, the preliminary study of a novel class of inhibitors of tubulin polymerization which possess novel temperature dependent activity is described. These studies seek to extend the use of tubulin as a therapeutic target to agents which possess temperature dependent activity.

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01121222

Subfile: Dictionary of Drugs, 1990;Dictionary of Steroids, 1991;Dictionary of Organic Compounds, 6th Edn., 1996;Dictionary of Pharmacological Agents, 1997

CHCD Acc. No: L-00049K0;L-00036J0;L-000096A20;L-00101X0

Unique Key: 00353351- -00

CHCD NAME: Liloeristone

Synonyms: 1-[4-(Dimethylamino)phenyl]-17-hydroxy-17-(3-hydroxy-1-propenyl)estradi-4,9-dien-3-one ; ZK 98734

Compound Type: Selected General Organics - Nonaromatic 19-norandrostane steroids (estranes) (C18); Pharmacological Agents - Abortifacients

Use/Importance: Abortifacient

Physical State: Pale-yellow foam

CAS Registry No: 97747-88-1

Molecular Formula: C₂₉H₃₇NO₃

Molecular Wt: 447.616

RTECS No.: KG2940000

Optical Rotation: +203.5 deg (CHCl₃) wavelength Na line

References:

01A GP 1985 3 347 126

01B CA 104 186715 (synth)

Data Tags: CAS Registry number; Molecular formula; Use/Importance; Physical State; Optical Rotation; Rtecs Reference

(7)

4/5/2

DIALOG(R) File 303:Chapman & Hall Chemical Database
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00433714

Subfile: Dictionary of Drugs, 1990;Dictionary of Steroids, 1991;Dictionary of Organic Compounds, 6th Edn., 1996;Dictionary of Pharmacological Agents, 1997

CHCD Acc. No: L-00049K0;L-00036J0;L-000096A20;L-00101X0

Unique Key: 00353351- -00

CHCD NAME: Liloeristone

Synonyms: 1-[4-(Dimethylamino)phenyl]-17-hydroxy-17-(3-hydroxy-1-propenyl)estradi-4,9-dien-3-one ; ZK 98734

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Molecular Wt: 447.616

RTECS No.: KG2940000

Optical Rotation: +203.5 deg (CHCl₃) wavelength Na line

References:

01A Ger. Pat. 1985 3 347 126

01B CA 104 186715 (synth)

Data Tags: CAS Registry number; Molecular formula; Use/Importance; Physical State; Optical Rotation; Rtecs Reference

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4/5/1

DIALOG(R) File 399:CA SEARCH(R)
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109110741 CA: 109(13)110741u PATENT
11.beta.- (4-Isopropenylphenyl)estra-4,9-dienes, procedure for their preparation, pharmaceutical preparations containing them, and their use as antigestagens

INVENTOR(AUTHOR): Ottow, Eckhard; Wiechert, Rudolf; Neef, Guenter; Beier, Sybille; Elger, Walter; Henderson, David

LOCATION: Fed. Rep. Ger.

ASSIGNEE: Schering A.-G.

PATENT: Germany Offen. ; DE 3625315 A1 DATE: 880128

APPLICATION: DE 3625315 (860725)

PAGES: 5 pp. CODEN: GWXXBX LANGUAGE: German CLASS: C07J-001/00A;
C07C-041/00B; A61K-031/565B; A61K-031/57B; A61K-031/575B

SECTION:

CA232003 Steroids

CA202XXX Mammalian Hormones

IDENTIFIERS: progesterone antagonist estradiene prepn, antigestagen
estradiene prepn

DESCRIPTORS:

Progestogens...

inhibitors, estradiene derivs.

Steroids, preparation...

prepn. of estradienes as antigestagens

CAS REGISTRY NUMBERS:

57-83-0 biological studies, antagonists to, estradiene derivs. as

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6888-79-5 Grignard reaction of, with epoxyestrenol deriv.

116196-34-0P 116229-17-5P prepn. and reaction of, in synthesis of
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116196-21-5P 116196-22-6P 116196-23-7P 116196-24-8P 116196-25-9P

116196-26-0P 116196-27-1P 116196-28-2P 116196-29-3P 116196-30-6P

116196-31-7P 116196-32-8P prepn. of, as antigestagen

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DIALOG(R) File 399:CA SEARCH(R)
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106129694 CA: 106(16)129694r JOURNAL

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11.beta.- (4-(dimethylamino)phenyl)-17.beta.-hydroxy-17.alpha.- (2-propenyl)e
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AUTHOR(S): Van Geerestein, V. J.; Kanters, J. A.; Kroon, J.

LOCATION: Lab. Kristal- Structuurchem., Rijksuniv. Utrecht, 3508 TB,
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JOURNAL: Acta Crystallogr., Sect. C: Cryst. Struct. Commun. DATE: 1987

VOLUME: C43 NUMBER: 2 PAGES: 319-22 CODEN: ACSCEE ISSN: 0108-2701

LANGUAGE: English

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CA232XXX Steroids

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methylaminophenyl hydroxy propenyl structure, propenylestradienone
structure

DESCRIPTORS:

8/5/9

DIALOG(R) File 399:CA SEARCH(R)

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72032135 CA: 72(7)32135a PATENT

3-Alkoxy-17.alpha.-propynylestra-1,3,5(10)-trien-17.beta.-ols

INVENTOR(AUTHOR): Galantay, Eugene E.

ASSIGNEE: Sandoz Ltd.

PATENT: Germany Offen. DE 1907330 DATE: 691023

APPLICATION: United States DATE: 680219

PAGES: 20 pp. CODEN: GWXXBX CLASS: C 07c; A 61k

SECTION:

CA832000 Steroids

IDENTIFIERS: estratrienols propynyl

DESCRIPTORS:

19-Norsteroids...

3-alkoxy

CAS REGISTRY NUMBERS:

24640-01-5P 24640-02-6P 24640-03-7P 24640-04-8P prep. of